Supplementary material

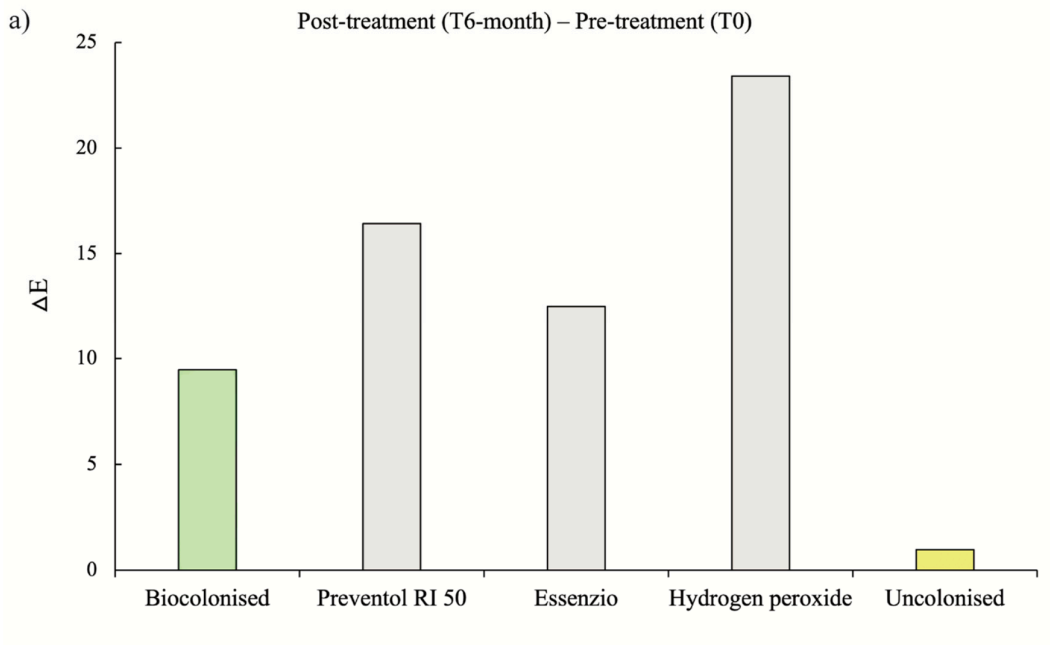

Figure S1. ΔE values before (t0) and after treatment (T6-month) of the different pilot areas.

ESI 1

1. Preventol RI 50

Benzalkonium chloride inventory was not present in ecoinvent [1], for this reason, it has been modelled by taking the Reaxys [2] database as a reference. In particular, it was synthesized via N,N-dimethylamino dodecane in the two following steps (Figure S1 and Table S1, synthesis of N,N-dimethylamino dodecane; and Figure S2 and Table S2, synthesis of Benzalkonyum chloride):

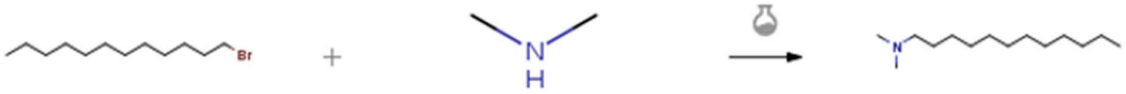

Figure S2: Synthesis of N,N-dimethylamino dodecane (Reaction ID: 647238; from [3]*)*

Table S1: Summarization of the stoichiometric calculation of Dimethylamine and Dodecanol mass involved in the synthesis of 1kg of N,N-dimethylamino dodecane.
**calculated by assuming a reaction rate of 98%* [3].
***Proxy process created ad hoc*

	n°mol	**MM**	**Mass** (kg/1mol)	**Mass** (kg/1kg of product)	**Proxy**
Dimethylamine	1	45.08	45.08	0.21	Dimethylamine {RER}| market for dimethylamine | APOS, U
Dodecan bromide	1	249.23	249.23	1.17	Dodecanol {GLO}| market for dodecanol | APOS, U
N,N-dimethylaminododecane	***1***	***213.41***	***213.41***	***1.02****	*_N,N-dimethylaminododecane {GLO}| production | APOS, U***

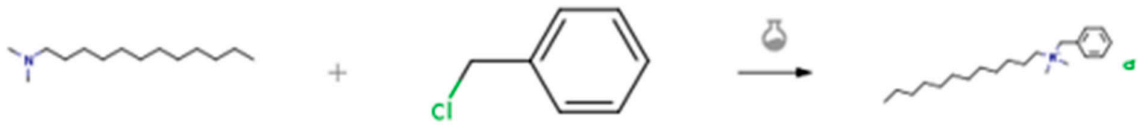

Figure S2: Synthesis of Benzalkonium chloride (Reaction ID: 604147; from [4]*)*

Table S2: Summarization of the stoichiometric calculation of N,N-dimethylamino dodecane and Benzyl chloride mass involved in the synthesis of 1kg of Benzalkonium chloride.
**calculated by assuming a reaction rate of 92.5%* [2].
***Proxy process created ad hoc*

	n°mol	**MM**	**Mass** (kg/1mol)	**Mass** (kg/1kg of product)	**Proxy**
N,N-dimethylaminododecane	1	213.41	213.41	0.68	*_N,N-dimethylaminododecane {GLO}| production | APOS, U*
Benzyl chloride	1	126.58	126.58	0.40	Benzyl chloride {RER}| market for benzyl chloride | APOS, U
Benzalkonium chloride	***1***	***339.99***	***339.99***	***1.08****	*_Benzalkonium chloride {GLO}| production | APOS, U***

Finally, since the Benzalkonyum chloride concentration was 10% (v/v), a new SimaPro process has been created by diluting 0.098 kg of Benzalkonyum chloride (ρ = 0.98 g/mL) in 0.902 kg of Ultrapure water (Table S3)

*Table S3: Preventol RI 50 dilution. *Proxy process created ad hoc.*

	Amount/Volume	**Unit**	**Proxy**
Benzalkonum chloride 10% v/v	1	L	_Benzalkonium chloride, 10% diluted {GLO}| production | APOS, U*
Benzalkonium chloride	0.098	kg	_Benzalkonium chloride {GLO}| production | APOS, U*
Water	0.902	kg	water, ultrapure {RER}| market for water, ultrapure | APOS, U

2. Essenzio (Oregano oil)

The inventory associated to oregano oil (ρ = 0.964 g/mL) production was drawn by [5]. The article proposes a system involving energy and solvents to extract the oil from oregano. Three strategies and two Scenarios were proposed to perform the extraction, but since Scenario 1 showed better extraction yields with respect to Scenario 2, it was selected as representative for our inventory. In the following model, only the energy consumption was considered for the estimation of the environmental impacts, since the solvents (i.e., supercritical CO_2) were always recovered with an efficiency ≈100%. Dried oregano from AGRIBALYSE [6] was introduced as input for the extraction. The impacts associated with the three strategies were finally averaged to estimate the energy consumption (Table S4). Thermal energy was assumed to be generated from Natural gas, the electricity mix was modeled according to the last available data in [7] regarding Italy.

Table S4: Energy consumption of the oregano oil extraction process [5]

	Supercritical fluid extraction (MJ/t)	**Solvent extraction** (MJ/t)	**Water Distillation Extraction** (MJ/t)	**Average** (MJ/t)
Heating	5.04E-01	4.59E-01	5.04E-01	**4.89E-01**
Cooling	5.35E-01	4.36E-01	5.02E-01	**4.91E-01**
Eletricity	1.77E-02	1.04E-02	9.52E-03	**1.25E-02**

3. Hydrogen Peroxide

The hydrogen peroxide 35% was included in the model according to ecoinvent process *Hydrogen peroxide, without water, in 35% solution state {RER}| market for hydrogen peroxide, without water, in 35% solution state | APOS, U* [1].

ESI 2

Table S5: Pedigree Matrix

	Beanzalkonium chloride		**N,N-dimethylaminododecane**		**Oregano oil**	
U1 (reliability)	1.2	3.32E-02	1.2	3.32E-02	1.2	3.32E-02
U2 (completeness)	1.05	2.38E-03	1.05	2.38E-03	1.05	2.38E-03
U3 (temporal c.)	1	0.00E+00	1	0.00E+00	1.1	9.08E-03
U4 (geographical c.)	1	0.00E+00	1	0.00E+00	1.1	9.08E-03
U5 (technological c.)	1.2	3.32E-02	1.2	3.32E-02	1.05	2.38E-03
Ub	1.05	2.38E-03	1.05	2.38E-03	1.05	2.38E-03
SD		1.31E+00		1.31E+00		1.27E+00

ESI 3

Table S6a: Environmental impacts estimated with ReCiPe 2016 LCIA method [8] *related to the application of the three alternatives (midpoint level, from GWP to MEP)*

	Liters	**GWP** (kg CO_2 eq)	**ODP** (kg CFC-11 eq)	**IRP** (kBq Co-60 eq)	**HOFP** (kg NO_x eq)	**PMFP** (kg PM2.5 eq)	**EOFP** (kg NO_x eq)	**TAP** (kg SO_2 eq)	**FEP** (kg P eq)	**MEP** (kg N eq)
Benzalkonium chloride	15	5.7E+00	1.2E-05	2.9E-01	1.1E-02	8.5E-03	1.1E-02	2.6E-02	2.9E-03	7.4E-03
SD		14.3%	24.4%	>50%	15.5%	16.7%	15.4%	17.2%	22.7%	26.9%
Oregano oil	15	1.7E+01	1.7E-04	5.7E-01	5.4E-02	4.2E-02	5.4E-02	2.0E-01	6.1E-03	4.0E-02
SD		8.0%	8.7%	10.4%	8.5%	8.6%	8.5%	8.6%	8.6%	8.7%
Hydrogen peroxide 35%	5	4.8E+00	1.7E-06	6.7E-01	8.0E-03	4.8E-03	8.1E-03	1.2E-02	2.2E-03	3.4E-04
SD		11%	14%	>50%	13%	15%	13%	15%	44%	15%

Table S6b: Environmental impacts estimated with ReCiPe 2016 LCIA method [8] *related to the application of the three alternatives (midpoint level, from TETP to WCP)*

	Liters	**TETP** (kg 1,4-DCB eq)	**FETP** (kg 1,4-DCB eq)	**METP** (kg 1,4-DCB eq)	**HTPc** (kg 1,4-DCB eq)	**HTPnc** (kg 1,4-DCB eq)	**LOP** (m^2a crop eq)	**SOP** (kg Cu eq)	**FFP** (kg oil eq)	**WCP** (m^3)
Benzalkonium chloride	15	9.1E-01	3.9E-02	3.3E-02	3.0E-03	5.7E-02	4.9E+00	1.7E-02	2.3E+00	6.1E-01
SD		37.2%	22.1%	23.4%	20.5%	31.4%	21.3%	32.7%	13.1%	>50%
Oregano oil	15	4.6E+00	2.0E-02	3.0E-02	3.4E-03	1.4E-01	2.8E+01	8.9E-02	3.8E+00	5.7E+00
SD		8.6%	8.6%	8.6%	9.1%	8.5%	8.7%	8.6%	7.8%	8.8%
Hydrogen peroxide 35%	5	1.0E+00	7.8E-03	1.2E-02	1.1E-03	5.7E-02	4.7E-01	1.7E-02	1.7E+00	3.1E-01
SD		73%	>50%	123%	23%	72%	37%	50%	12%	>50%

Table S6c: Environmental impacts estimated with ReCiPe 2016 LCIA method [8] *related to the application of the three alternatives (endpoint level)*

	Liters	**Human health** (mPts)	**Ecosystem quality** (mPts)	**Resources Scarcity** (mPts)
Benzalkonium chloride	15	225.57	20.04	0.29
SD		>50%	34%	29%
Oregano oil	15	6.2E+02	1.1E+02	1.2E+01
SD		8.9%	9.1%	9.1%
Hydrogen peroxide 35%	5	2.7E+02	8.7E+00	1.9E-01
SD		25%	37%	26%

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